

Calculation of parity nonconservation in neutral ytterbium

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We use configuration interaction and many-body perturbation theory techniques to calculate spin-independent and spin-dependent parts of the parity nonconserving amplitudes of the transitions between the $6s^2\ ^1S_0$ ground state and the $6s5d\ ^3D_1$ excited state of ^{171}Yb and ^{173}Yb . The results are presented in a form convenient for extracting spin-dependent interaction constants (such as, e.g., anapole moment) from the measurements.

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I. INTRODUCTION

The use of atomic ytterbium to study parity nonconservation (PNC) in atoms was first suggested by DeMille [1]. The measurements are in progress at Berkeley and after years of hard work [2–5] the first results of PNC measurements are finally reported [6]. As it was expected the PNC in ytterbium is strongly enhanced, being two orders of magnitude larger than in cesium [7]. The cesium PNC experiment together with its interpretation [8–10] in terms of nuclear weak charge provides the best current atomic test of the standard model (see, also a review [11]). It is also the only measurement of the nuclear *anapole moment* which is produced by the PNC nuclear forces [12]. The extraction of the weak nuclear charge from the PNC measurements relies on atomic calculations. The interpretation of the PNC measurements in ytterbium similar to what was done for cesium is not possible due to limitations of atomic theory. Ytterbium has complicated electron structure and calculations for it on the same level of accuracy as for cesium are not possible now and in foreseen future. The aims of the PNC measurements in Yb are different [6]: (i) to study the ratio of the PNC amplitudes for different isotopes, and (ii) to measure nuclear spin-dependent PNC effects, such as the effect of nuclear anapole moment. The study of the PNC for a chain of isotopes does not require atomic calculations and can deliver useful information about either neutron distribution or new physics beyond standard model (see, e.g. [14–17]). The extraction of the anapole moment from the measurements does require atomic calculations, however, high theoretical accuracy is not critical here.

Ytterbium is a very good candidate for both types of the experimental studies. It has seven stable isotopes with large difference in neutron numbers $\Delta N_{\max} = 8$. Two of the isotopes, ^{171}Yb and ^{173}Yb , have non-zero nuclear spin provided by valence neutron. This is especially interesting since it allows one to measure the strength of the neutron-nucleus PNC potential [12] (the anapole moment has been measured only for the ^{133}Cs nucleus which has valence proton).

Calculations of the spin-independent PNC in ytter-

bium were performed in Refs. [1, 18, 19]. Calculations of the spin-dependent PNC were reported in [20, 21]. The results of [20, 21] for the spin-dependent PNC amplitudes are presented as tables of reduced matrix elements of the spin-dependent weak interaction for different hyperfine transitions. This, in our view, leads to some difficulties in interpretation. Reduced matrix elements (RME) are very convenient for intermediate calculations. However, presenting final results in a form of RME may lead to confusion due to their unnatural symmetry properties:

$$\langle F_a, a || \hat{H} || F_b, b \rangle = (-1)^{F_a - F_b} \langle F_b, b || \hat{H} || F_a, a \rangle^*. \quad (1)$$

Here F_a is the total momentum of the state a , asterisk means complex conjugation which in the case of PNC amplitudes means the change of sign. There is an apparent disagreement between the signs of different RME in [20] and [21]. The most likely explanation for this in our view is that the authors of [20] and [21] presented different RME, say $\langle a || \hat{H} || b \rangle$ in [20] and $\langle b || \hat{H} || a \rangle$ in [21]. At least all sign differences follow strictly the rule (1).

Strictly speaking, the sign of an amplitude is not defined (since a wave function may be multiplied by an arbitrary phase factor), only the ratio of two amplitudes between the same states has definite sign. Neither of the work [20, 21] provides a link between the spin-dependent (SD) PNC amplitudes and spin-independent (SI) PNC amplitudes calculated earlier in [18, 19]. This means that it is hard to say whether the spin-dependent effects increase or decrease a particular PNC amplitude. In other words, the sign of the spin-dependent interaction constants, such as the anapole moment, cannot be extracted from the measurements when using the calculations of [20] or [21] and no additional assumptions (note that the apparent disagreement between the signs of the amplitudes in [20] and [21] shows that any guesswork about the relative signs of the SI and SD amplitudes is unreliable).

To avoid this problem, in present paper both spin-independent and spin-dependent PNC amplitudes are calculated simultaneously using the same procedure and the same wave functions. In this approach the relative sign of the amplitudes is fixed. This allows for unambiguous determination of the sign of the spin-dependent

contribution. The constant of the spin-dependent interaction can be expressed via the ratio of the two amplitudes. This brings an extra advantage of more accurate interpretation of the measurements. The accuracy of the calculations for the ratio of the PNC amplitudes is higher than that for each of the amplitudes. This is because the amplitudes are very similar in nature and most of the theoretical uncertainty cancels out in the ratio.

II. THEORY

Hamiltonian describing parity-nonconserving electron-nuclear interaction can be written as a sum of spin-independent (SI) and spin-dependent (SD) parts (we use atomic units: $\hbar = |e| = m_e = 1$):

$$\begin{aligned} H_{\text{PNC}} &= H_{\text{SI}} + H_{\text{SD}} \\ &= \frac{G_F}{\sqrt{2}} \left(-\frac{Q_W}{2} \gamma_5 + \frac{\kappa}{I} \boldsymbol{\alpha} \mathbf{I} \right) \rho(\mathbf{r}), \end{aligned} \quad (2)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$ and γ_5 are the Dirac matrices, \mathbf{I} is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1. The strength of the spin-dependent PNC interaction is proportional to the dimensionless constant κ which is to be found from the measurements. There are three major contributions to κ arising from (i) electromagnetic interaction of atomic electrons with nuclear *anapole moment*, (ii) electron-nucleus spin-dependent weak interaction, and (iii) combined effect of spin-independent weak interaction and magnetic hyperfine interaction (see, e.g. [11]). In this work we do not distinguish between different contributions to κ and present the results in terms of total κ which is the sum of all possible contributions.

Within the standard model the weak nuclear charge Q_W is given by [13]

$$Q_W \approx -0.9877N + 0.0716Z. \quad (3)$$

Here N is the number of neutrons, Z is the number of protons.

The PNC amplitude of an electric dipole transition between states of the same parity $|i\rangle$ and $|f\rangle$ is equal to:

$$\begin{aligned} E1_{fi}^{\text{PNC}} &= \sum_n \left[\frac{\langle f | \mathbf{d} | n \rangle \langle n | H_{\text{PNC}} | i \rangle}{E_i - E_n} \right. \\ &\quad \left. + \frac{\langle f | H_{\text{PNC}} | n \rangle \langle n | \mathbf{d}_q | i \rangle}{E_f - E_n} \right], \end{aligned} \quad (4)$$

where $\mathbf{d} = -e \sum_i \mathbf{r}_i$ is the electric dipole operator, $|a\rangle \equiv |J_a F_a M_a\rangle$ and $\mathbf{F} = \mathbf{I} + \mathbf{J}$ is the total angular momentum.

Applying the Wigner-Eckart theorem we can express the amplitudes via reduced matrix elements

$$\begin{aligned} E1_{fi}^{\text{PNC}} &= (-1)^{F_f - M_f} \begin{pmatrix} F_f & 1 & F_i \\ -M_f & q & M_i \end{pmatrix} \\ &\quad \times \langle J_f F_f || d_{\text{PNC}} || J_i F_i \rangle. \end{aligned} \quad (5)$$

Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found e.g. in Refs. [22] and [23]. For the SI amplitude we have

$$\begin{aligned} \langle J_f, F_f || d_{\text{SI}} || J_i, F_i \rangle &= (-1)^{I + F_i + J_f + 1} \\ &\times \sqrt{(2F_f + 1)(2F_i + 1)} \begin{Bmatrix} J_i & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \\ &\times \sum_n \left[\frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || H_{\text{SI}} || J_i \rangle}{E_i - E_n} \right. \\ &\quad \left. + \frac{\langle J_f || H_{\text{SI}} || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_f - E_n} \right] \\ &\equiv c(F_f, J_f, F_i, J_i) E'_{fi}. \end{aligned} \quad (6)$$

Here $c(F_f, J_f, F_i, J_i)$ is the angular coefficient and the sum over n , E'_{fi} does not depend on F_f or F_i :

$$\begin{aligned} E' &= \sum_n \left[\frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || H_{\text{SI}} || J_i \rangle}{E_i - E_n} \right. \\ &\quad \left. + \frac{\langle J_f || H_{\text{SI}} || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_f - E_n} \right]. \end{aligned} \quad (7)$$

For the SD PNC amplitude we have

$$\begin{aligned} \langle J_f, F_f || d_{\text{SD}} || J_i, F_i \rangle &= \frac{G_F}{\sqrt{2}} \kappa \\ &\times \sqrt{(I + 1)(2I + 1)(2F_i + 1)(2F_f + 1)/I} \\ &\times \sum_n \left[(-1)^{J_f - J_i} \begin{Bmatrix} J_n & J_i & 1 \\ I & I & F_i \end{Bmatrix} \begin{Bmatrix} J_n & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \right. \\ &\quad \times \frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || \boldsymbol{\alpha} \rho || J_i \rangle}{E_n - E_i} \\ &\quad \left. + (-1)^{F_f - F_i} \begin{Bmatrix} J_n & J_f & 1 \\ I & I & F_f \end{Bmatrix} \begin{Bmatrix} J_n & J_i & 1 \\ F_i & F_f & I \end{Bmatrix} \right. \\ &\quad \left. \times \frac{\langle J_f || \boldsymbol{\alpha} \rho || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_n - E_f} \right]. \end{aligned} \quad (8)$$

In the case of the $^1S_0 - \rightarrow ^3D_1$ transition these expressions can be significantly simplified. Substituting $F_i = I$, $J_i = 0$, $F_f = I, I \pm 1 \equiv F$, $J_f = 1$, $J_n = 1$ we have for the PNC amplitudes (z -components) E_{F_i, F_f} of the transitions between specific hfs states of ^{171}Yb ($I = 1/2$)

$$E_{\frac{1}{2}, \frac{1}{2}, z} = -\frac{1}{3} E' Q_W - \sqrt{\frac{2}{27}} E'' \kappa, \quad (9)$$

$$E_{\frac{1}{2}, \frac{3}{2}, z} = \sqrt{\frac{2}{9}} E' Q_W - \sqrt{\frac{1}{27}} E'' \kappa. \quad (10)$$

Similar expressions for ^{173}Yb ($I = 5/2$) are

$$E_{\frac{5}{2}, \frac{3}{2}, z} = -\sqrt{\frac{4}{45}} E' Q_W - \sqrt{\frac{98}{3375}} E'' \kappa, \quad (11)$$

$$E_{\frac{5}{2}, \frac{5}{2}, z} = -\sqrt{\frac{5}{21}} E' Q_W - \sqrt{\frac{2}{315}} E'' \kappa, \quad (12)$$

$$E_{\frac{5}{2}, \frac{7}{2}, z} = \sqrt{\frac{2}{21}} E' Q_W - \sqrt{\frac{1}{63}} E'' \kappa. \quad (13)$$

Here E'' is the part of the SD PNC amplitude which is independent on F_i and F_f :

$$E'' = \frac{G_F}{\sqrt{2}} \sum_n \left[\frac{\langle J_f || \mathbf{d} || n, J_n \rangle \langle n, J_n || \boldsymbol{\alpha} \rho || J_i \rangle}{E_n - E_i} - \frac{\langle J_f || \boldsymbol{\alpha} \rho || n, J_n \rangle \langle n, J_n || \mathbf{d} || J_i \rangle}{E_n - E_f} \right]. \quad (14)$$

Note that if at least two PNC amplitudes are measured then the value of \varkappa can be expressed via the ratio E''/E' of the calculated SD and SI PNC amplitudes. This ratio is much less sensitive to numerical uncertainties than each of the amplitudes. The amplitudes are very similar. Therefore, a greater part of the numerical uncertainty cancels out in the ratio. For example, if amplitudes (9) and (10) are measured then

$$\varkappa = \sqrt{3} \frac{\sqrt{2}R + 1}{S(R - \sqrt{2})}, \quad (15)$$

where $R = E_{\frac{1}{2}, \frac{1}{2}, z} / E_{\frac{1}{2}, \frac{3}{2}, z}$ and $S = E'' / (E' Q_W)$. The ratio of theoretical amplitudes E''/E' is significantly more stable in the calculations than each of the amplitudes.

III. CALCULATIONS

We consider ytterbium as an atom with two valence electrons above closed shells and use the combination of the configuration interaction and many-body perturbation theory (CI+MBPT, [24]) to perform the calculations. The calculations are very similar to our previous calculations of ytterbium polarizabilities [25]. Below we briefly describe the procedure emphasizing some minor differences.

A. CI+MBPT method

The effective CI+MBPT Hamiltonian for two valence electrons has the form

$$\hat{H}^{\text{eff}} = \hat{h}_1(r_1) + \hat{h}_1(r_2) + \hat{h}_2(r_1, r_2), \quad (16)$$

where \hat{h}_1 is the single-electron part of the relativistic Hamiltonian

$$\hat{h}_1 = c\hat{\alpha}\mathbf{p} + (\hat{\beta} - 1)m_e c^2 - \frac{Ze^2}{r} + V^{N-2} + \hat{\Sigma}_1, \quad (17)$$

and \hat{h}_2 is the two-electron part of the Hamiltonian

$$\hat{h}_2(r_1, r_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \hat{\Sigma}_2(r_1, r_2). \quad (18)$$

In these equations, $\hat{\alpha}$ and $\hat{\beta}$ are the conventional Dirac matrices, V^{N-2} is the Dirac-Hartree-Fock (DHF) potential of the closed-shell atomic core ($N-2 = 68, Z = 70$),

and $\hat{\Sigma}$ is the correlation operator. It represents terms in the Hamiltonian arising due to virtual excitations from atomic core (see Ref. [24, 26] for details). $\hat{\Sigma} \equiv 0$ corresponds to the standard CI method. $\hat{\Sigma}_1$ is a single-electron operator. It represents a correlation interaction (core-polarization) of a particular valence electron with the atomic core. $\hat{\Sigma}_2$ is a two-electron operator. It represents screening of the Coulomb interaction between the two valence electrons by the core electrons. We calculate $\hat{\Sigma}$ in the second order of the MBPT. We use a B-spline technique [27] to construct a complete set of single-electron orbitals. We use 40 B-splines in a cavity of radius $R = 40 a_B$ and calculate the eigenstates of the V^{N-2} DHF Hamiltonian up to the maximum value of the angular momentum $l_{\text{max}} = 5$. The same basis is used in computing $\hat{\Sigma}$ and in constructing the two-electron states for the valence electrons. 40 out of 60 lowest-energy states for every l up to $l_{\text{max}} = 5$ are used to calculate $\hat{\Sigma}$ and 16 lowest states above the core are used for every l up to $l_{\text{max}} = 4$ to construct the two-electron states.

The two-electron valence states are found by solving the eigenvalue problem,

$$\hat{H}^{\text{eff}} \Psi_v = E_v \Psi_v, \quad (19)$$

using the standard CI techniques. Calculated and experimental energies of a few lowest-energy states of Yb can be found in Ref. [25]. The pure *ab initio* energies are already close to the experimental values. However, for improving the accuracy further, we re-scale the correlation operator $\hat{\Sigma}_1$ by replacing $\hat{\Sigma}_1$ in the effective Hamiltonian (16) in each partial wave $s, p_{1/2}, p_{3/2}, \dots$ by $f_a \hat{\Sigma}_1$. The rescaling factors are $f_s = 0.875$, $f_p = 1.268$, $f_d = 0.935$, and $f_f = 1$. These values are chosen to fit the experimental spectrum of Yb. Some differences in scaling parameters compare to what was used in Ref. [25] is due to the fact that in present work we have fitted exactly the energy of the $^1P_1^o$ state while in [25] we fitted the energy of the $^3P_1^o$ state.

B. Dalgarno-Lewis and RPA methods

Matrix elements are found with the random-phase approximation (RPA) [28, 29]

$$E1_{vw} = \langle \Psi_v || \hat{f} + \delta V^{N-2} || \Psi_w \rangle, \quad (20)$$

where δV^{N-2} is the correction to the core potential due to core polarization by an external field \hat{f} . In present calculations \hat{f} represents either external electric field, SI weak interaction or SD PNC interaction.

Computing PNC requires summing over a complete set of two-electron states (see, e.g. Eq. (4)). We use the Dalgarno-Lewis method [30] for the summation. In this method, a correction $\delta \Psi_v$ to the two-electron wave function of the state v is introduced and the amplitude is reduced to

$$A_{vw} = \langle \delta \Psi_v || \hat{f}_1 || \Psi_w \rangle. \quad (21)$$

TABLE I: Magnetic dipole hyperfine structure constants A (MHz) for the $^3P_1^o$ and $^1P_1^o$ states of ^{171}Yb , comparison with experiment.

| State | Calculations | Experiment ^a |
|-----------|--------------|-------------------------|
| $^3P_1^o$ | 4460 | 3958 |
| $^1P_1^o$ | -819 | -1094 |

^aReference [31].

The correction $\delta\Psi_v$ is found by solving the system of linear inhomogeneous equations

$$(\hat{H}^{\text{eff}} - E_v)\delta\Psi_v = -(\hat{f}_2 + \delta V^{N-2})\Psi_v. \quad (22)$$

Here \hat{f}_1 and \hat{f}_2 are electric dipole and PNC interaction operators ($\hat{f}_1 = \mathbf{d}$, $\hat{f}_2 = H_{\text{PNC}}$ or vice versa).

C. Accuracy of the calculations

Accuracy of very similar calculations of polarizabilities of ytterbium were studied in detail in our previous work [25] and were found to be about 5%. However, we cannot claim the same accuracy for present calculations due to two important differences. First, there is a resonance contribution to the PNC amplitude involving the $^1P_1^o$ state. Energy interval between the 3D_1 and $^1P_1^o$ states is very small. Its experimental values is just 579 cm^{-1} . The term in (4) involving the $^1P_1^o$ state gives more than 80% of the total PNC amplitude. Even very accurate calculations may give significantly different value of small energy interval which would lead to large error in the PNC amplitude. One way around this problem is to separate the resonance term from the rest of the sum and use the experimental energy for the denominator. We use a technically more simple procedure. We have rescaled the correlation operator $\hat{\Sigma}$ to fit the interval exactly. As a result, the contribution of the error in the energy denominator to the error in the amplitude is small.

Another important difference of present calculations from those of Ref. [25] is that we need to calculate matrix elements of weak interaction which are sensitive to the wave functions on short distances. A way to test the wave functions on short distances is to calculate hyperfine structure (hfs) constants.

Calculated and experimental values of the magnetic dipole hyperfine structure constants A for the $^3P_1^o$ and $^1P_1^o$ states of ^{171}Yb are presented in Table I. The first calculated hfs constant is larger than the experimental one by 13%, the second is smaller by 25%. The reason for the calculated hyperfine constant of the $^1P_1^o$ state to differ significantly from the the experimental value is the same as for the electric dipole transition amplitude between this and ground state - the admixture of the $4f^{13}5d6s^2$ ($7/2, 3/2$) $_1^o$ state at $E = 28857 \text{ cm}^{-1}$ (see Ref. [25] for details). This admixture is small. However, it

TABLE II: PNC amplitudes (z -components) for the $|6s^2, ^1S_0, F_1\rangle \rightarrow |6s5d, ^3D_1, F_2\rangle$ transitions in ^{171}Yb and ^{173}Yb in units of $E'Q_W$ and $10^{-9}iea_0$.

| A | I | F_1 | F_2 | PNC amplitude | |
|-----|-----|-------|-------|----------------------------------|---------------------------|
| | | | | units: $E'Q_W$ | units: $10^{-9}iea_0$ |
| 171 | 0.5 | 0.5 | 0.5 | $-(1/3)(1 - 0.0161\kappa)$ | $6.15(1 - 0.0161\kappa)$ |
| | | 0.5 | 1.5 | $\sqrt{2/9}(1 + 0.0081\kappa)$ | $-8.70(1 + 0.0081\kappa)$ |
| 173 | 2.5 | 2.5 | 1.5 | $-\sqrt{4/45}(1 - 0.0111\kappa)$ | $5.61(1 - 0.0111\kappa)$ |
| | | 2.5 | 2.5 | $-\sqrt{5/21}(1 - 0.0032\kappa)$ | $9.18(1 - 0.0032\kappa)$ |
| | | 2.5 | 3.5 | $\sqrt{2/21}(1 + 0.0079\kappa)$ | $-5.81(1 + 0.0079\kappa)$ |

can change hfs of the $^1P_1^o$ state significantly due to the large hfs in the admixed state. In contrast, it cannot change that much the weak matrix element between the $^1P_1^o$ and $4f^{14}5d6s$ 3D_1 states. This is because the transition between the $4f^{13}5d6s^2$ and the $4f^{14}5d6s$ 3D_1 states in zero approximation is the $6s \rightarrow 4f$ transition and corresponding weak matrix element is zero. Therefore, poor accuracy for the hfs of the $^1P_1^o$ state is not a good indicator for the accuracy of the PNC calculations. A 13% error in the hfs of the $^3P_1^o$ state gives a more realistic estimate for the uncertainty.

We stress that the uncertainty in the ratio of SD and SI PNC amplitudes (E''/E') is significantly lower. Tests show that this ratio is three to five times less sensitive to the variation of the calculation procedure than each of the amplitudes. We believe that 10% is a reasonable estimate for the theoretical uncertainty for this ratio.

IV. RESULTS

Calculations give the following value of the spin-independent PNC amplitude of the $^1S_0 \rightarrow ^3D_1$ transition in ytterbium:

$$E_z^{\text{SI-PNC}} = 1.123 \times 10^{-11} Q_W iea_0. \quad (23)$$

This corresponds to the following value of the reduced matrix element

$$E' = 1.945 \times 10^{-11} iea_0. \quad (24)$$

The electron (F -independent) part of the reduced matrix element of the spin-dependent PNC amplitude is found to be

$$E'' = 3.648 \times 10^{-11} iea_0, \quad (25)$$

The effect of different nuclear size for ^{171}Yb and ^{173}Yb is only 0.1% for both SI and SD PNC amplitudes. It is neglected in (23), (24) and (25). We use Fermi-type distribution for nuclear density ρ with nuclear radius $R_N = 6.35 \text{ fm}$ for ^{171}Yb and $R_N = 6.37 \text{ fm}$ for ^{173}Yb [32].

The ratios of the SD and SI PNC amplitudes are

$$E''/(E'Q_W) = -0.0198(20) \text{ for } ^{171}\text{Yb}, \quad (26)$$

$$E''/(E'Q_W) = -0.0194(20) \text{ for } ^{173}\text{Yb}. \quad (27)$$

The difference in these values is due to different weak nuclear charge Q_W ($Q_W = -94.75$ for ^{171}Yb and $Q_W = -96.72$ for ^{173}Yb). The difference is within numerical uncertainty.

The results for the specific PNC amplitudes between different hyperfine structure states of ^{171}Yb and ^{173}Yb are presented in Table II. These results are obtained by substituting (24) and (25) into (9), (10), (11), (12) and (13). The numerical factors before \varkappa are proportional to (E''/E') . The theoretical uncertainty for these factors is about 10%. The expressions from the table or equations (9), (10), (11), (12), (13) together with (24) and (25) can be used to extract the value of \varkappa from the measurements. For example, for ^{171}Yb Eq. (15) becomes

$$\varkappa = 88(9) \frac{1 + \sqrt{2}R}{(\sqrt{2} - R)}. \quad (28)$$

A. Comparison with other calculations

Calculations of the spin-independent part of the PNC amplitude for ytterbium were performed before in Refs. [1, 18, 19]. The spin-dependent amplitudes were calculated before in Refs. [20, 21]. It is convenient to compare the results in terms of E' (7) and E'' (14) since these values are the same for all hfs transitions. Refs. [1, 18, 19] present the values of the z -component of the SI PNC amplitude. Refs. [20, 21] present reduced matrix elements of the SD PNC interaction for each hfs transition. Corresponding values of E' and E'' can be easily extracted from this data using formulas of present paper. The absolute values of the amplitudes are presented in Table III. We have excellent agreement for E' with DeMille [1] and Porsev *et al* [18] while the result of Das [19] is about 30% smaller. We have good agreement with both Porsev *et al* [21] and Singh and Das [20] for E'' . The difference between Ref. [21] and our result is 12% which is within our uncertainty. The difference between our results for E'' and those of Ref. [20] is even smaller. But this is probably accidental. Note however that we agree with Singh and Das [20] on small, practically negligible change of E'' from ^{171}Yb to ^{173}Yb while Porsev *et al* [21] report a 3% increase. Such increase has no physical explanation and must be a numerical effect. In our experience such effect can be a result of just one RPA iteration after a change of nuclear radius from ^{171}Yb to ^{173}Yb . Further iterations kill the difference. However, it is up to the authors of [21] to explain their results.

Note again that in Table III we present only the absolute values of the amplitudes, ignoring their signs. This is because the sign of an amplitude is not fixed and has no physical meaning. However, the relative sign of the SI and SD PNC amplitudes is not arbitrary. The SD dependent part of the PNC amplitude must either increase or decrease the transition amplitude depending on the sign of \varkappa . It is important to know the relative sign of the amplitudes to be able to extract the sign of \varkappa from the mea-

TABLE III: Spin-independent (E') and spin-dependent (E'') parts of the PNC amplitude (reduced matrix elements) for the $|6s^2, ^1S_0\rangle \rightarrow |6s5d, ^3D_1\rangle$ transition in ytterbium, comparison with other calculations. The signs of the amplitudes are omitted.

| | E' | E'' ($10^{-11}iea_0$) | |
|---------------------|-------------------|---------------------------|-------------------|
| | $10^{-11}iea_0$ | ^{171}Yb | ^{173}Yb |
| DeMille [1] | 1.9 | | |
| Porsev <i>et al</i> | 1.97 ^a | 4.13 ^b | 4.27 ^b |
| Singh and Das | 1.33 ^c | 3.68 ^d | 3.67 ^d |
| This work | 1.95 | 3.65 | 3.64 |

^aRef. [18], ^bRef. [21], ^cRef. [19], ^dRef. [20].

surements. To fix the relative sign of the two PNC amplitudes one should calculate them using the same wave functions. This is how it is done in present work (see Table II and formulas (9), (10), (11), (12), (13)). Another important advantage of the simultaneous calculation of both amplitudes is that \varkappa can be expressed via the ratio of the amplitudes. This ratio has much smaller theoretical uncertainty than each of the amplitudes (see previous section for discussion).

Unfortunately, both previous calculations of the SD PNC amplitude in Yb [20, 21] do not compare their results with the earlier calculations of the SI PNC amplitudes [18, 19] which could be performed using different wave functions. This leads to the uncertainty of the relative signs and larger errors in the ratios of the SI and SD amplitudes which are needed to extract the value of \varkappa from the measurements.

B. Comparison with experiment

The result of the measurement of the PNC amplitude of the $^1S_0 \rightarrow ^3D_1$ transition in ^{174}Yb reported in [6] reads

$$|E^{\text{PNC}}| = 8.7(1.4) \times 10^{-10}ea_0. \quad (29)$$

Assuming a 13% theoretical uncertainty and substituting weak nuclear charge $Q_W = -97.71$ we get from (23) the following theoretical value for the amplitude

$$|E^{\text{PNC}}| = 11.0(1.4) \times 10^{-10}ea_0. \quad (30)$$

The values of (29) and (30) agree within the declared uncertainty.

To measure the constant of spin-dependent PNC interaction (\varkappa) more accurate measurements are needed for ^{171}Yb or ^{173}Yb . The work is in progress at Berkeley [6].

V. CONCLUSION

We present simultaneous calculation of the spin-independent and spin-dependent PNC amplitudes of the

$6s^2 \ ^1S_0 \rightarrow 6s5d \ ^3D_1$ transition in ytterbium. The results are to be used for accurate interpretation of future measurements in terms of the parameter of the spin-dependent PNC interaction κ . Both, sign and value of κ can be determined. Theoretical uncertainty is at the level of 10%.

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